IUCLID

Data Set

Existing Chemical	:	ID: 68515-40-2
Memo	:	HPV Chemical
CAS No.	:	68515-40-2
TSCA Name	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Synonym	:	Phthalic acid, benzyl alkyl(C7-C8) ester

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	07.12.2006
Revision date	:	
Date of last update	:	06.07.2006
Number of pages	:	25
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freetext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)

117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)

16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)

68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)

68515-45-7 1,2,-benzenedicarboxylic acid, dinonyl ester, branched and

linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :

Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -48 - -35 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Remark	:	Manufacturer's data or handbook value. The data from this structure contribute to the range of values used to characterize this substance. There were no data on purity.
Test substance	:	Read across data for CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters. The data range represents 1,2-benzenedicarboxylic acid, dinonyl ester, branched and linear (CAS No. 68515-45-7) and butylbenzyl phthalate ester (CAS No. 85-68-7).
Reliability	:	(2) valid with restrictions Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed database.
Flag	:	Critical study for SIDS endpoint
15.05.2006		(9)

Value	:	90 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle. The SMILES notation used in the calculation: CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Reliability	:	(3) invalid
15.05.2006		(4)

2.2 BOILING POINT

Value	:	427 °C at 1013 hPa
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown. The SMILES notation used in the calculation: CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

15.05.2006 (4)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.000000579 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain. The SMILES notation used in the calculation: CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

06.07.2006 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	6.74 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Method	:	Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard. The SMILES notation used in the calculation:

CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2

Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

31.05.2006 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	.00847 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 8.54.
The SMILES notation used in the calculation:
CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2

Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

31.05.2006 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.0000000000167 cm³/(molecule*sec)
Degradation	:	50 % after 7.7 hour(s)
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson. The SMILES notation used in the calculation: CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2
Remark	:	50% degradation after 7.69 hrs or 0.64 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

31.05.2006 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	1.4 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al. The SMILES notation used in the calculation: CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property

estimation.

Test substance : CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
31.05.2006 (4)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	368.48
Temperature	25° C
Log Kow	6.74
Water Solubility	0.00847 g/m3
Vapor Pressure	0.0000579 Pa

Melting Point = -42C (taken as midpoint between range: -48 and -35)

Result : Using the Mackay Level I calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
31.05.2006 (5)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III

Year :

Remark : Physicochemical data used in the calculation:

Parameter Value w/ Units

Molecular Weight 368.48
Temperature 25° C
Log Kow 6.74
Water Solubility 0.00847 g/m3
Vapor Pressure 0.0000579 Pa
Melting Point = -42C (taken as midpoint between range: -48 and -35)

Emissions rates used in the calculation:

Compartment Rate (kg/hr)

Air 1000
Water 1000
Soil 1000

Half-lives used in the calculation:

Compartment Half-life (hr)

Air 15.4a
Water 120b
Soil 420c
Sediment 420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from: Exxon Biomedical Sciences, Inc. (1995), Staples et al. (1997), and Boethling (2000):

Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Staples, C., D. Peterson, T. Parkerton and W. Adams (1997). The Environmental Fate of Phthalate Esters: A literature Review. Chemosphere 35:667-749.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters:

Compartment % Distribution
Air 1.2
Water 9.2

		Soil 69.9
		Sediment 19.7
Test substance	:	CAS #68515-40-2; 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

31.05.2006 (5)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 1000 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	other
Year	:	1975
GLP	:	yes
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters; CAS # 68515-40-2
Method	:	Method/Guideline - U.S. EPA-600/3-75-009, Methods for Acute Toxicity tests with Fish, Macroinvertebrates and Amphibians. 1975 Statistical methods - NA
Result	:	No mortality was observed. No test substance insolubility was noted in report. Fish mean total length = 32.7 mm, mean wet weight = 0.47 g, organism loading was not calculated. Nominal test concentrations: Loading Level (mg/L) Mortality (96h) Control 0 100 0 180 0 320 0 560 0 1000 0
Test condition	:	The test treatments were prepared by individually mixing the appropriate amount of test substance with 10 ml of acetone and adding it directly to the test chambers. The control also received 10 ml of solvent. One replicate was prepared for each test treatment and control. The test was performed in 5-gallon glass vessels containing 15 L of dilution water. The dilution water was filter well water. Each treatment vessel contained 10 fish. Test temperature = 12 +/- 1 Deg C. The pH range was 7.5 to 7.9. The dissolved oxygen ranged from 8.0 to 8.9 mg/L. Fish were obtained from Fender's Fish Hatchery in Baltic, Ohio. Nominal test concentrations: Loading Level (mg/L) Control, 100, 180, 320, 560, 1000
Test substance	:	Benzyl, C7-9 branched and linear phthalate (CAS# 68515-40-2)
Conclusion	:	Test substance is non-toxic to fish at or below its water solubility level.
Reliability	:	(2) valid with restrictions There was limited information on the water quality parameters.
Flag	:	Critical study for SIDS endpoint

31.05.2006 (2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)

Unit	:	mg/l
LC50	:	4.5 calculated
Analytical monitoring	:	no
Method	:	other
Year	:	1975
GLP	:	yes
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters; CAS # 68515-40-2
Method	:	Method/Guideline - U.S. EPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975 Statistical methods - Moving average angle, Probit or Bionomial
Result	:	Test organisms in the 1.0 and 1.8 mg/L loading levels were observed "clumped" together at 48 hours. Nominal test concentrations: Loading Level (mg/L) Mortality (48 h) Control 0 Solvent Control 0 1.0 0 1.8 2 3.2 6 5.6 13 10.0 20 Units-LC50 Value - 4.5 mg/L (CI of 3.5 to 5.9) based upon nominal loading levels.
Test condition	:	Test treatments were prepared by adding the test substance with acetone directly to the test treatments. Two replicates of ten organisms were tested per treatment except the controls, which were tested with one replicate. Test vessels were 250 ml beakers with 200 ml of test solution. The dilution water was well water. Test temperature = 20 +/- 1 Deg C. The pH ranged from 7.8 to 8.1 during the study. Dissolved oxygen ranged from 8.9 to 9.3 mg/L. Dilution water hardness was 240 mg/L and Alkalinity was 360 mg/L. Daphnia were <24 hours old and obtained from in-house stock. Lighting was 16 hours light and 8 hours dark (no intensity reported). Nominal test concentrations: Loading Level (mg/L) Control, Solvent Control, 1.0, 1.8, 3.2, 5.6, 10.0
Test substance	:	Benzyl, C7-9 branched and linear phthalate (CAS# 68515-40-2)
Reliability	:	(3) invalid Test organisms were reported as clumped together. Observed mortality resulted from physical effects.
Flag	:	Critical study for SIDS endpoint

06.07.2006 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 674 measured/nominal
Limit test	:	
Analytical monitoring	:	no
Method	:	other
Year	:	1971
GLP	:	yes

Test substance : other TS: 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters; CAS # 68515-40-2

Method : Method/Guideline - EPA, Algal Assay Procedure: Bottle Test, 1971.
Test type - Static Acute
Statistical methods-NA

Result : In-vivo chlorophyll a, was measured daily. Both cell numbers and in-vivo chlorophyll a, measured at termination.
Chlorophyll a measured using a Turner filter flourometer. Cell counts performed via a hemacytometer.

% Difference at 96 hr relative to control:

Loading Level (mg/L)	Chlorophyll a	Cell #
Control	---	---
56	-8	-6
100	-12	-6
180	-18	-19
320	-20	-24
560	-55	-63
1000	-61	-69

Units-ppm
Value - EC50 = 674 mg/L, based upon in-vivo chlorophyll a measurement.
EC50 = 521 mg/L, based upon cell number.

Test condition : The appropriate amount of test substance was added directly to algal growth medium (control and diluent) to form individual treatment concentrations. The test was performed in 125 ml flasks. The initial algal concentration was 3.0x104 cells per ml.

Lighting = 4,000 lux, Test temperature=24+/-1 Deg C. The pH range was 7.2 to 7.6. Algal culture stock obtained from U.S. EPA Environmental Research Laboratory, Corvallis, Oregon.

Nominal test concentrations:
control, 56, 100, 180, 320, 560, and 1,000 mg/L.

Test substance : Benzyl, C7-9 Branched and Linear Phthalate (CAS# 68515-40-2)

Reliability : (3) invalid
No final cell counts reported. Limited details on test treatment preparation in report. Test is considered invalid because of the presence of "Globules" of test material observed in all test flasks during the study.

Flag : Critical study for SIDS endpoint
31.05.2006 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 15800 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: Undiluted test material administered
Doses	:	
Method	:	other
Year	:	1976
GLP	:	no
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters; CAS # 68515-40-2
Test condition	:	The undiluted test material was fed by stomach tube to a single group of rats at a dose level of 15800 mg/kg. Five rats (3 male, 2 female) were used. The rats were observed for toxic signs and sacrificed after 14 days.
Test substance	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters (CAS # 68515-40-2)
Conclusion	:	The compound was found to be non-lethal by oral ingestion in male and female rats at a dose of 15800 mg/kg.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

06.07.2006 (6)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	> - 7940 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	3
Vehicle	:	other: Undiluted test material administered
Doses	:	
Method	:	other
Year	:	1976
GLP	:	no
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters; CAS # 68515-40-2
Remark	:	No animals died at either dose level. Toxic signs reported as reduced appetite and activity for 1 to 3 days. All rabbits appeared normal at necropsy.
Test condition	:	The undiluted compound was applied at doses of 5010 and 7940 mg/kg to the closely clipped, intact skin of rabbits. The treated areas were covered with plastic strips and animals held in wooden stocks for up to 24 hours, after which they were held in individual cages. The rabbits were observed

for toxic signs daily for 14 days. Surviving animals were sacrificed after 14 days and observed for internal macroscopic abnormalities.

Test substance	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters (CAS # 68515-40-2)
Conclusion	:	The test substance was considered practically non-toxic by dermal exposure in male and female rabbits.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

06.07.2006 (7)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Test concentration	:	0.01, 0.04, 0.2, 1.0, 3.0, and 10.0 ul/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1982
GLP	:	yes
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters; CAS # 68515-40-2
Method	:	Statistical analysis was performed on the results after transforming values to log10. Analysis included Bartlett's test for homogeneity of variance and comparison to controls with a t-test. Dose-response was evaluated with regression analysis and significance of the response evaluated by a t-test.
Remark	:	The substance was not mutagenic at doses < 10 mg/plate in Salmonella strains TA98, TA100, TA1535, TA1537 and TA1538 in plate incorporation assays with or without metabolic activation. No microbial toxicity was observed in any of the five strains at 10 mg/plate with or without metabolic activation, although levels of 3 ug/plate and higher exceeded the solubility of the test material.
Test condition	:	Positive control chemicals were sodium nitrite, 9-aminoacridine, and 4-nitroquinoline-N-oxide (without S9); or benzo(a)pyrene, 2-acetylaminofluorene, and 2-aminoanthracene (with S9); the solvent control was DMSO. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA100 was conducted with and without microsomal activation to determine the highest dose level. The plate incorporation tests were conducted in all strains with and without activation.
Test substance	:	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl esters

(CAS # 68515-40-2)

Conclusion : The test substance was not mutagenic in all strains tested.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
06.07.2006 (8)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Analytical Bio Chemistry Laboratories, Inc (ABC) (1979). Static Acute Bioassay No. 23040-B, for Monsanto Chemical Company, St. Louis, MO, USA.

(2) Analytical Bio Chemistry Laboratories, Inc (ABC) (1980). Static Acute Bioassay No. 25427, for Monsanto Chemical Company, St. Louis, MO, USA.

(3) EG&G, Bionomics Marine Research Laboratory (1979). Freshwater Alga Toxicity Test with Selenastrum capricornutum. Report No. BP-79-2-20 for Monsanto Chemical Company, St. Louis, MO, USA.

(4) Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.

(5) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

(6) Monsanto Company (1976). Acute oral toxicity with Santicizer 261. Unpublished report.

(7) Monsanto Company (1976). Minimum lethal dose by skin adsorption in rabbits with Santicizer 261. Unpublished report.

(8) Monsanto Research Corporation (1982). Salmonella mutagenicity assay of Santicizer 261. Unpublished report.

(9) Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. Chemosphere 35, 667-749.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

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10.3 RISK ASSESSMENT